Broad comp search.

```
Connecting via Winsock to STN


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LOGINID:ssptayvv1621

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2


* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS  1           Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2           "Ask CAS" for self-help around the clock
 NEWS  3  AUG 09   INSPEC enhanced with 1898-1968 archive
 NEWS  4  AUG 28   ADISCTI Reloaded and Enhanced
 NEWS  5  AUG 30   CA(SM)/CAplus(SM) Austrian patent law changes
 NEWS  6  SEP 11   CA/CAplus enhanced with more pre-1907 records
 NEWS  7  SEP 21   CA/CAplus fields enhanced with simultaneous left and right
                   truncation
 NEWS  8  SEP 25   CA(SM)/CAplus(SM) display of CA Lexicon enhanced
 NEWS  9  SEP 25   CAS REGISTRY(SM) no longer includes Concord 3D coordinates
 NEWS 10  SEP 25   CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
 NEWS 11  SEP 28   CEABA-VTB classification code fields reloaded with new
                   classification scheme
 NEWS 12  OCT 19   LOGOFF HOLD duration extended to 120 minutes
 NEWS 13  OCT 19   E-mail format enhanced
 NEWS 14  OCT 23   Option to turn off MARPAT highlighting enhancements available
 NEWS 15  OCT 23   CAS Registry Number crossover limit increased to 300,000 in
                   multiple databases
 NEWS 16  OCT 23   The Derwent World Patents Index suite of databases on STN
                   has been enhanced and reloaded
 NEWS 17  OCT 30   CHEMLIST enhanced with new search and display field
 NEWS 18  NOV 03   JAPIO enhanced with IPC 8 features and functionality
 NEWS 19  NOV 10   CA/CAplus F-Term thesaurus enhanced
 NEWS 20  NOV 10   STN Express with Discover! free maintenance release Version
                   8.01c now available
 NEWS 21  NOV 13   CA/CAplus pre-1967 chemical substance index entries enhanced
                   with preparation role
 NEWS 22  NOV 20   CAS Registry Number crossover limit increased to 300,000 in
                   additional databases
 NEWS 23  NOV 20   CA/CAplus to MARPAT accession number crossover limit increased
                   to 50,000
 NEWS 24  NOV 20   CA/CAplus patent kind codes will be updated
 NEWS 25  DEC 01   CAS REGISTRY updated with new ambiguity codes
 NEWS 26  DEC 11   CAS REGISTRY chemical nomenclature enhanced

 NEWS EXPRESS  NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8
 NEWS X25      X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that
specific topic.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 09:02:54 ON 14 DEC 2006

=> file reg
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 0.21 0.21

FILE 'REGISTRY' ENTERED AT 09:03:07 ON 14 DEC 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 13 DEC 2006 HIGHEST RN 915360-23-5
DICTIONARY FILE UPDATES: 13 DEC 2006 HIGHEST RN 915360-23-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10540749-broader.str

L1 STRUCTURE UPLOADED

=> s l1
SAMPLE SEARCH INITIATED 09:03:26 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 13857 TO ITERATE

14.4% PROCESSED 2000 ITERATIONS 31 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

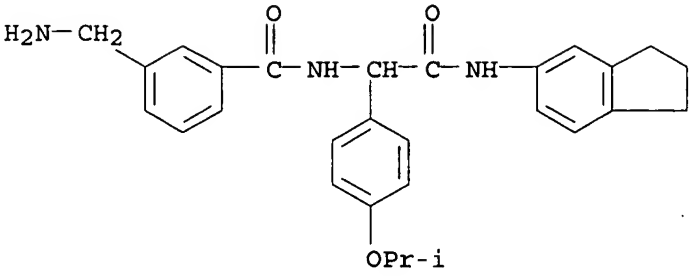
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 270088 TO 284192
PROJECTED ANSWERS: 3416 TO 5174

L2 31 SEA SSS SAM L1

=> d l2 scan

L2 31 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzeneacetamide, α-[[3-(aminomethyl)benzoyl]amino]-N-(2,3-dihydro-1H-inden-5-yl)-4-(1-methylethoxy)- (9CI)

MF C28 H31 N3 O3
CI COM

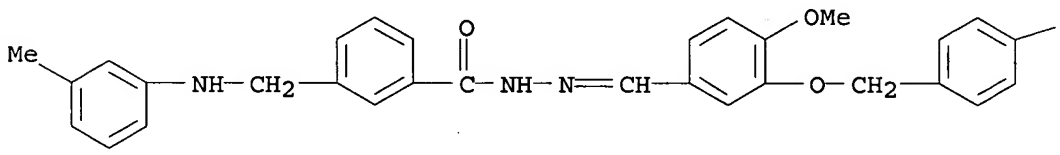


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L2 31 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzoic acid, 3-[[(3-methylphenyl)amino]methyl]-, [[4-methoxy-3-[(4-nitrophenyl)methoxy]phenyl]methylene]hydrazide (9CI)
MF C30 H28 N4 O5

PAGE 1-A

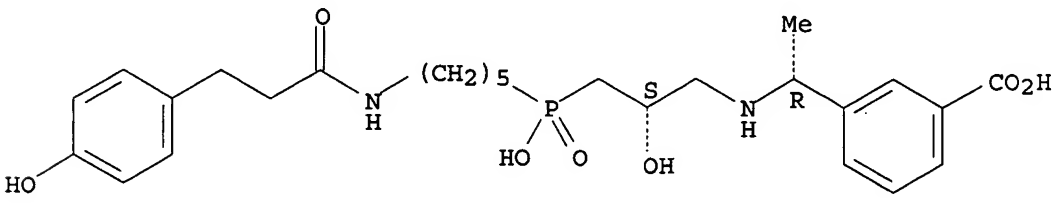


PAGE 1-B

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzoic acid, 3-[1-[[2-hydroxy-3-[hydroxy[5-[[3-(4-hydroxyphenyl)-1-oxopropyl]amino]pentyl]phosphinyl]propyl]amino]ethyl]-, [S-(R*,S*)]- (9CI)
MF C26 H37 N2 O7 P

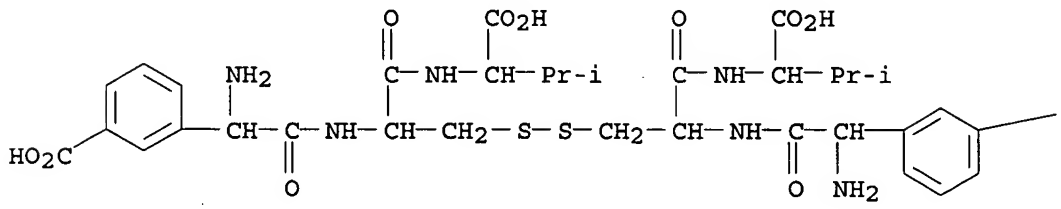
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN D-Valine, 2-(3-carboxyphenyl)glycyl-L-cysteinyl-, bimol. (2→2')-disulfide (9CI)
MF C34 H44 N6 O12 S2

PAGE 1-A

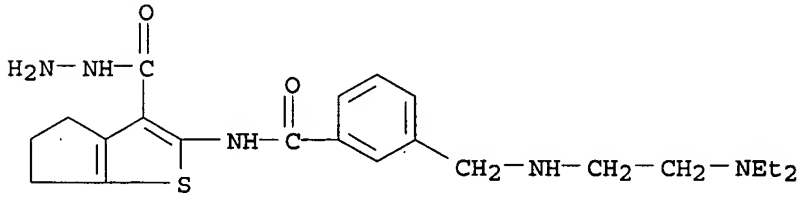


PAGE 1-B

—CO_2H

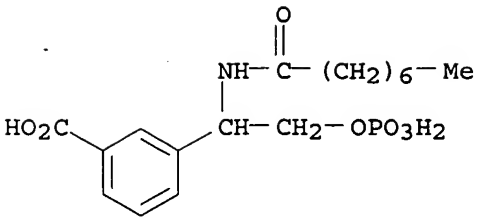
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 4H-Cyclopenta[b]thiophene-3-carboxylic acid, 2-[[3-[[[2-(diethylamino)ethyl]amino]methyl]benzoyl]amino]-5,6-dihydro-, hydrazide (9CI)
MF C22 H31 N5 O2 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 31 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzoic acid, 3-[1-[(1-oxooctyl)amino]-2-(phosphonooxy)ethyl]-, trisodium salt (9CI)
MF C17 H26 N O7 P . 3 Na



3 Na

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> s l1 full
FULL SEARCH INITIATED 09:04:34 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 279585 TO ITERATE

100.0% PROCESSED 279585 ITERATIONS 3239 ANSWERS
SEARCH TIME: 00.00.02

L3 3239 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	167.82	168.03

FILE 'CAPLUS' ENTERED AT 09:04:44 ON 14 DEC 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 14 Dec 2006 VOL 145 ISS 25
FILE LAST UPDATED: 13 Dec 2006 (20061213/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l3 and friedel
757 L3
17141 FRIEDEL
L4 1 L3 AND FRIEDEL

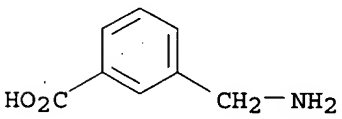
=> d l4 ibib abs hitstr

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:324185 CAPLUS

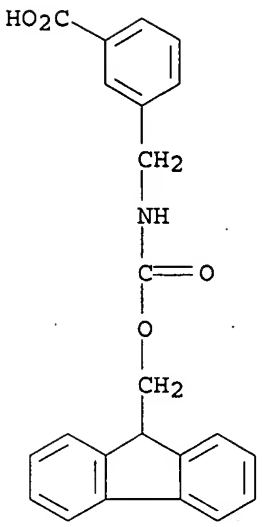
DOCUMENT NUMBER: 120:324185
TITLE: Design and Synthesis of a Biologically Active Antibody Mimic Based on an Antibody-Antigen Crystal Structure
AUTHOR(S): Smythe, M. L.; von Itzstein, M.
CORPORATE SOURCE: Victorian College of Pharmacy, Monash University, Parkville, 3052, Australia
SOURCE: Journal of the American Chemical Society (1994), 116(7), 2725-33
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The crystal structure of an N9 sialidase (antigen)-NC41 (antibody) complex was used to design a low mol. weight cyclopeptide that mimics the binding function of the macromol. antibody. The components of recognition between the antibody and the protein antigen have been analyzed from the energy-refined crystal complex. From this anal., four amino acid residues on the antibody binding surface, which make direct contact with the active-site loop 368-370 of the antigen, were identified as contributing the majority of the binding energy of the protein. The designed target cyclo(Phe-Amb-Glu-Asp-Asn) [Amb = 3-(aminomethyl)benzoic acid], a constrained cyclic peptide that mimics the receptor-bound conformation of these amino acids, was prepared and found to inhibit N9 sialidase activity with a Ki of 1 + 10-4 M.

IT 2393-20-6P, 3-(Aminomethyl)benzoic acid
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and fluorenylmethoxycarbonylation of)
RN 2393-20-6 CAPLUS
CN Benzoic acid, 3-(aminomethyl)- (9CI) (CA INDEX NAME)



IT 155369-11-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and solid-phase peptide coupling reactions of, in preparation of
cyclopeptide antibody mimic)
RN 155369-11-2 CAPLUS
CN Benzoic acid, 3-[[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]methyl]- (9CI) (CA INDEX NAME)



```
=> s l3 and acylation
          757 L3
        59127 ACYLATION
L5         19 L3 AND ACYLATION

=> d l5 ibib abs hitstr

L5   ANSWER 1 OF 19  CAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:        2006:333345  CAPLUS
DOCUMENT NUMBER:         144:350709
TITLE:                   Pyrazolopyrimidines as protein kinase B inhibitors,
                         their preparation, pharmaceutical compositions, and
                         use in therapy
INVENTOR(S):             Maier, Thomas; Zuelch, Armin; Ciossek, Thomas; Baer,
                         Thomas; Beckers, Thomas
PATENT ASSIGNEE(S):      Altana Pharma AG, Germany
SOURCE:                  PCT Int. Appl., 114 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:           Patent
LANGUAGE:                English
FAMILY ACC. NUM. COUNT:  1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
     ---------------      ----   --------    --------------------    --------
     WO 2006027346         A2    20060316    WO 2005-EP54366         20050905
     WO 2006027346         A3    20060803
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
             LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,
             NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,
             SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,
             ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
PRIORITY APPLN. INFO.:                       EP 2004-104283      A  20040906
OTHER SOURCE(S):         MARPAT 144:350709
```

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to pyrazolopyrimidine derivs. I, which are inhibitors of protein kinase B (PKB)/Akt. In compds. I, R1 is (un)substituted aryl or (un)substituted heteroaryl; R2 is H, halo, or C1-4 alkyl; R3 is selected from (un)substituted amino-C1-4 alkyl, heterocyclyl-C1-4 alkyl, (un)substituted Ph, (un)substituted phenyl-C1-4 alkyl, (un)substituted heteroaryl, etc.; and R4 is H or halo; including salts thereof. The invention also relates to the preparation of I, pharmaceutical compns. comprising one or more compds. of formula I together with a pharmaceutically acceptable carrier or diluent, as well as to the use of the compns. for the treatment, prevention, or amelioration of benign or malignant neoplasia, such as cancer. Deprotonation of 4-methoxybut-3-en-2-one followed by acylation with 4-bromobenzoyl chloride gave pentenedione II, which underwent heterocyclization with thiosemicarbazide, S-methylation, and oxidation resulting in the formation of sulfonylpyrazolopyrimidine III. Compound III was substituted with tert-Bu N-(4-aminophenyl)carbamate followed by deprotection, amidation with N-Boc-4-(2-aminoethyl)benzoic acid, and deprotection to give the hydrochloride salt of pyrazolopyrimidine IV. Five compds. of the invention, e.g., IV, inhibit Akt1 with IC50 values below 4.03 μM and exhibit antiproliferative/cytotoxic activity with IC50 values below 16.9 μM and 13.6 μM in assays using MCF7 and MDA468 cancer cell lines, resp.

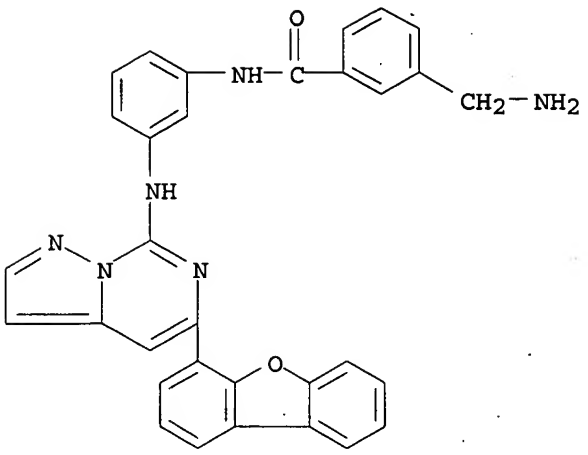
IT 881215-02-7P, 3-Aminomethyl-N-[3-((5-(Dibenzofuran-4-yl)pyrazolo[1,5-c]pyrimidin-7-yl)amino)phenyl]benzamide trifluoroacetate
881215-06-1P, 3-Aminomethyl-N-[4-((5-(Dibenzofuran-4-yl)pyrazolo[1,5-c]pyrimidin-7-yl)amino)phenyl]benzamide trifluoroacetate
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of pyrazolopyrimidines as protein kinase B inhibitors)

RN 881215-02-7 CAPLUS

CN Benzamide, 3-(aminomethyl)-N-[3-[[5-(4-dibenzofuranyl)pyrazolo[1,5-c]pyrimidin-7-yl]amino]phenyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 881215-01-6
CMF C32 H24 N6 O2



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CRN 76-05-1
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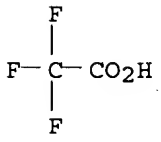
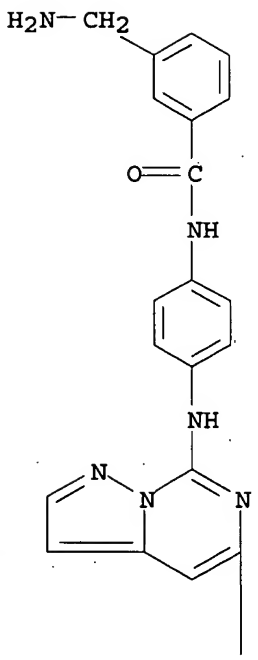


RN 881215-06-1 CAPLUS
CN Benzamide, 3-(aminomethyl)-N-[4-[[5-(4-dibenzofuranyl)pyrazolo[1,5-c]pyrimidin-7-yl]amino]phenyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

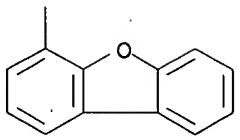
CM 1

CRN 881215-05-0
CMF C32 H24 N6 O2

PAGE 1-A

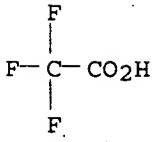


PAGE 2-A



CM 2

CRN 76-05-1
CMF C2 H F3 O2



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=> s l3 and aromatic substitution
           757 L3
        231823 AROMATIC
        259602 SUBSTITUTION
          2102 AROMATIC SUBSTITUTION
                 (AROMATIC(W)SUBSTITUTION)
L6           0 L3 AND AROMATIC SUBSTITUTION

=> s l3 and substitution
           757 L3
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        259602 SUBSTITUTION
L7          28 L3 AND SUBSTITUTION

=> s l7 or l5
L8          45 L7 OR L5

=> s l8 not py > 2003
       3632143 PY > 2003
L9          31 L8 NOT PY > 2003

=> d l9 ibib abs hitstr

L9   ANSWER 1 OF 31  CAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         2003:478576  CAPLUS
DOCUMENT NUMBER:          139:175717
TITLE:                    Recognition and resistance in TEM β-lactamase
AUTHOR(S):                Wang, Xiaojun; Minasov, George; Blazquez, Jesus;
                          Caselli, Emilia; Prati, Fabio; Shoichet, Brian K.
CORPORATE SOURCE:         Department of Pharmaceutical Chemistry, University of
                          California San Francisco, San Francisco, CA, 94143,
                          USA
SOURCE:                   Biochemistry (2003), 42(28), 8434-8444
                          CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER:                American Chemical Society
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
AB   Developing antimicrobials that are less likely to engender resistance has
     become an important design criterion as more and more drugs fall victim to
     resistance mutations. One hypothesis is that the more closely an
     inhibitor resembles a substrate, the more difficult it will be to develop
     resistant mutations that can at once disfavor the inhibitor and still
     recognize the substrate. To investigate this hypothesis, 10
     transition-state analogs, of greater or lesser similarity to substrates,
     were tested for inhibition of TEM-1 β-lactamase, the most widespread
     resistance enzyme to penicillin antibiotics. The inhibitors were also
     tested against four characteristic mutant enzymes: TEM-30, TEM-32, TEM-52,
     and TEM-64. The inhibitor most similar to the substrate, compound 10, was
     the most potent inhibitor of the WT enzyme, with a Ki value of 64 nM.
     Conversely, compound 10 was the most susceptible to the TEM-30 (R244S)
     mutant, for which inhibition dropped by over 100-fold. The other
     inhibitors were relatively impervious to the TEM-30 mutant enzyme. To
     understand recognition and resistance to these transition-state analogs,
     the structures of four of these inhibitors in complex with TEM-1 were
     determined by x-ray crystallog. These structures suggest a structural basis
     for distinguishing inhibitors that mimic the acylation
     transition state and those that mimic the deacylation transition state;
     they also suggest how TEM-30 reduces the affinity of compound 10. In cell
     culture, this inhibitor reversed the resistance of bacteria to ampicillin,
     reducing min. inhibitory concns. of this penicillin by between 4- and
     64-fold, depending on the strain of bacteria. Notwithstanding this
     activity, the resistance of TEM-30, which is already extant in the clinic,
     suggests that there can be resistance liabilities with substrate-based
     design.
IT   497258-67-0D, complexes with TEM-1 β-lactamase
     RL: PRP (Properties)
        (crystal structure of TEM-1 β-lactamase-transition state analog
        complexes)
RN   497258-67-0  CAPLUS
CN   Benzoic acid, 3-[(R)-borono[(2-thienylacetyl)amino]methyl]- (9CI)  (CA
     INDEX NAME)

Absolute stereochemistry.  Rotation (-).
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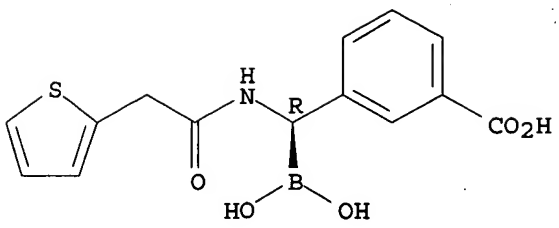
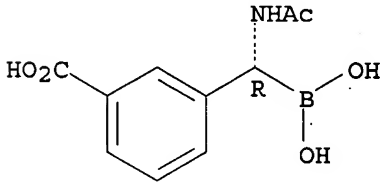


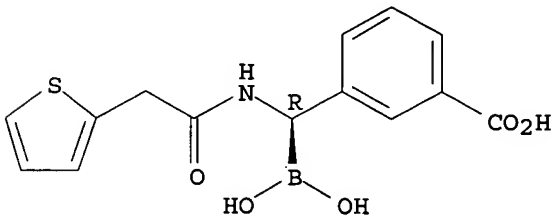
IT 497258-66-9 497258-67-0 497258-68-1
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(transition state analog recognition and inhibition by TEM β-lactamase mutants in relation to antibiotic resistance)
RN 497258-66-9 CAPLUS
CN Benzoic acid, 3-[(R)-(acetylamino)boronomethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



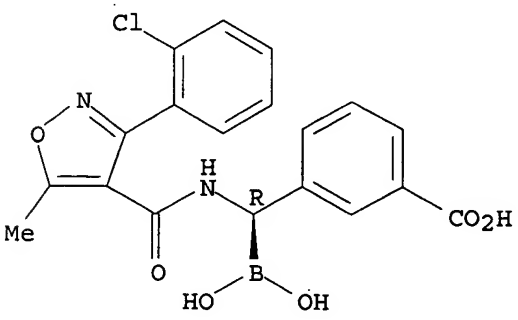
RN 497258-67-0 CAPLUS
CN Benzoic acid, 3-[(R)-borono[(2-thienylacetyl)amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 497258-68-1 CAPLUS
CN Benzoic acid, 3-[(R)-borono[[[3-(2-chlorophenyl)-5-methyl-4-isoxazolyl]carbonyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	33.01	201.04

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.25	-2.25

FILE 'REGISTRY' ENTERED AT 09:12:41 ON 14 DEC 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 13 DEC 2006 HIGHEST RN 915360-23-5
DICTIONARY FILE UPDATES: 13 DEC 2006 HIGHEST RN 915360-23-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

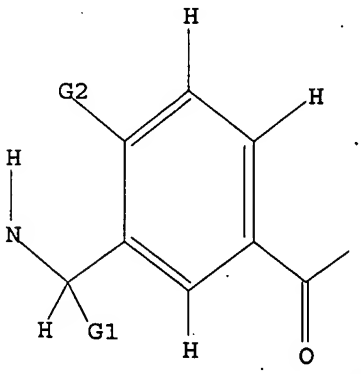
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10540749-broader2.str

L10 STRUCTURE UPLOADED

=> d l10
L10 HAS NO ANSWERS
L10 STR



G1 H,Me,Et,n-Pr,i-Pr,n-Bu,i-Bu
G2 H,X

Structure attributes must be viewed using STN Express query preparation.

=> s l10
SAMPLE SEARCH INITIATED 09:13:24 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2433 TO ITERATE

82.2% PROCESSED 2000 ITERATIONS 6 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 45702 TO 51618
PROJECTED ANSWERS: 6 TO 307

L11 6 SEA SSS SAM L10

=> s l10 full
FULL SEARCH INITIATED 09:13:29 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 49225 TO ITERATE

100.0% PROCESSED 49225 ITERATIONS 117 ANSWERS
SEARCH TIME: 00.00.01

L12 117 SEA SSS FUL L10

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	167.38	368.42

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.25

FILE 'CAPLUS' ENTERED AT 09:13:36 ON 14 DEC 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 14 Dec 2006 VOL 145 ISS 25
FILE LAST UPDATED: 13 Dec 2006 (20061213/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l12
L13 49 L12

```
=> acylation and l13
ACYLATION IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> s l13 and acylation
         59127 ACYLATION
L14          0 L13 AND ACYLATION

=> s l13 not py > 2002
       4688838 PY > 2002
L15         14 L13 NOT PY > 2002

=> d l15 ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 14 ANSWERS - CONTINUE? Y/(N):y

L15  ANSWER 1 OF 14  CAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         2002:823424  CAPLUS
DOCUMENT NUMBER:          139:6655
TITLE:                    Highly potent inhibitors of TNF-α production.
                          Part I. Discovery of new chemical leads and Their
                          structure-Activity relationships
AUTHOR(S):                Matsui, Toshiaki; Kondo, Takashi; Nishita, Yoshitaka;
                          Itadani, Satoshi; Nakatani, Shingo; Omawari,
                          Nagashige; Sakai, Masaru; Nakazawa, Shuichi; Ogata,
                          Akihito; Mori, Hideaki; Terai, Kouichiro; Kamoshima,
                          Wataru; Ohno, Hiroyuki; Obata, Takaaki; Nakai, Hisao;
                          Toda, Masaaki
CORPORATE SOURCE:         Fukui Research Institute, Ono Pharmaceutical Co.,
                          Ltd., Sakai, Fukui, 913-8638, Japan
SOURCE:                   Bioorganic & Medicinal Chemistry (2002), 10(12),
                          3757-3786
                          CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER:                Elsevier Science Ltd.
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
OTHER SOURCE(S):          CASREACT 139:6655
AB   Discovery of new chemical leads of inhibitors for TNF-α production starting
     from the chemical modification of 2-(octanoylamino)-2-phenylethyl disodium
     phosphate (I) is reported.  Further biol. studies of I to disclose the
     site of its action strongly suggested that I inhibits LPS-induced
     TNF-α expression in the liver and spleen of mice.
     Structure-activity relationships (SARs) are also discussed and full
     details including the chemical are reported.
IT   532986-93-9P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of alkylamino aryl disodium phosphates and their
        structure-activity relationships as highly potent inhibitors of
        TNF-α production)
RN   532986-93-9  CAPLUS
CN   Octanamide, N-[1-[3-(diazoacetyl)phenyl]-2-(phenylmethoxy)ethyl]- (9CI)
     (CA INDEX NAME)
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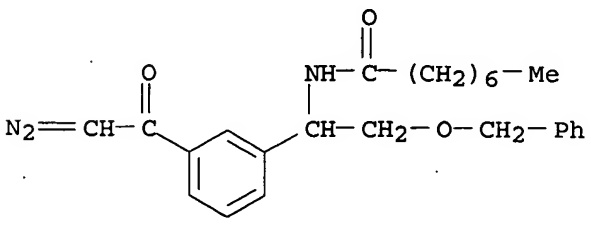


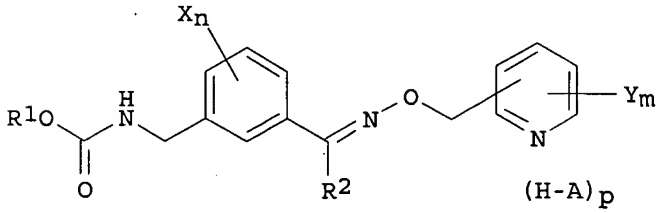
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:615570 CAPLUS
DOCUMENT NUMBER: 137:140441
TITLE: Preparation of iminooxymethylpyridine compounds and agricultural or horticultural fungicides
INVENTOR(S): Fukumoto, Shunichiro; Shibayama, Atsushi; Shibata, Masaru; Yonekura, Norihisa; Takagaki, Makiichi; Miura, Ichiro; Nagayama, Kouzou
PATENT ASSIGNEE(S): Kumiai Chemical Industry Co., Ltd., Japan; Ihara Chemical Industry Co., Ltd.
SOURCE: PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002062759	A1	20020815	WO 2002-JP792	20020131

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: JP 2001-26827 A 20010202
OTHER SOURCE(S): MARPAT 137:140441
GI



I

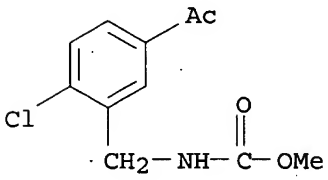
AB Novel benzylideneiminooxymethylpyridine compound derivs. having the following general formula (I; wherein X represents halogeno, C1-6 alkyl, C1-6 alkoxy, C1-6 haloalkyl, or C1-6 haloalkoxy; Y represents halogeno, C1-6 alkyl, or C1-6 alkoxy; p is 0, 1/2, or 1; m and n each independently is an integer of 0 to 4; R1 represents C1-6 alkyl; R2 represents hydrogen, C1-6 alkyl, or C1-6 haloalkyl; and H-A represents an acid substance) are prepared and also disclosed are agricultural or horticultural fungicides containing the derivs. I as the active ingredient. Thus, 18.9 g K2CO3 and 13.9 g 2-chloromethyl-6-methylpyridine hydrochloride were added to a solution of 10.0 g N-[2-chloro-5-(1-hydroxyiminoethyl)benzyl]carbamic acid Me ester in 100 mL DMF and stirred at 90-100° for 8 h to give 8.2 g N-[2-chloro-5-[1-(6-methylpyridin-2-ylmethoxy)iminoethyl]benzyl]carbamic acid Me ester (II). II at 500 ppm completely controlled Erysiphe graminis in wheat seedlings.

IT 325155-92-8P, N-(2-Chloro-5-acetylbenzyl)carbamic acid methyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation of iminooxymethylpyridine compds. and agricultural or horticultural fungicides)

RN 325155-92-8 CAPLUS

CN Carbamic acid, [(5-acetyl-2-chlorophenyl)methyl]-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:836782 CAPLUS

DOCUMENT NUMBER: 136:118413

TITLE: Anti-Helicobacter pylori Agents. 5. 2-(Substituted guanidino)-4-arylthiazoles and Aryloxazole Analogues

AUTHOR(S): Katsura, Yousuke; Nishino, Shigetaka; Inoue, Yoshikazu; Sakane, Kazuo; Matsumoto, Yoshimi; Morinaga, Chizu; Ishikawa, Hirohumi; Takasugi, Hisashi

CORPORATE SOURCE: Medicinal Chemistry Research Laboratories and Medicinal Biology Research Laboratories, Fujisawa Pharmaceutical Company Ltd., Yodogawa-ku, Osaka, 532-8514, Japan

SOURCE: Journal of Medicinal Chemistry (2002), 45(1), 143-150
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

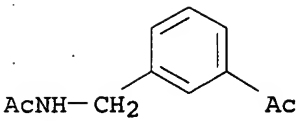
OTHER SOURCE(S): CASREACT 136:118413

AB To extend the SAR study of guanidinothiazoles as a structurally novel class of anti-H. pylori agents, a series of 2-(substituted guanidino)-4-arylthiazoles and some 4-aryloxazole analogs were synthesized and evaluated for antimicrobial activity against H. pylori. Some of them were also subjected to H2 antagonist and gastric antisecretory assays. Several arylthiazoles were identified as potent anti-H. pylori agents, and of these, a thienylthiazole derivative exhibited the strongest activity (MIC = 0.0065 μg/mL) among the compds. obtained in our guanidinothiazole studies. Although the thienylthiazole derivative was void of H2 antagonist activity, a pyridylthiazole derivative had both potent anti-H. pylori and H2 antagonist activities. On the other hand, no attractive activities were found in pyrimidyl, oxazolyl, isoxazolyl, imidazolyl, and oxadiazolylthiazole derivs. The anti-H. pylori activity of the aryloxazole analogs was weaker than those of the corresponding arylthiazole derivs., though they had potent H2 antagonist activity.

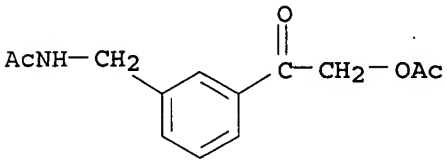
IT 149917-34-0 170634-23-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of guanidinoarylthiazoles and aryloxazoles and their antimicrobial activity against H. pylori., H2 antagonist activity, and gastric antisecretory assays)

RN 149917-34-0 CAPLUS

CN Acetamide, N-[(3-acetylphenyl)methyl]- (9CI) (CA INDEX NAME)



RN 170634-23-8 CAPLUS
CN Acetamide, N-[[3-[(acetyloxy)acetyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

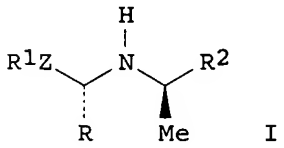


REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:241760 CAPLUS
DOCUMENT NUMBER: 134:280612
TITLE: Preparation of 1-arylethylamines as calcium receptor ligands
INVENTOR(S): Van Wagenen, Bradford C.; Moe, Scott T.; Balandrin, Manuel F.; Delmar, Eric G.; Nemeth, Edward F.
PATENT ASSIGNEE(S): NPS Pharmaceuticals, Inc., USA
SOURCE: U.S., 142 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

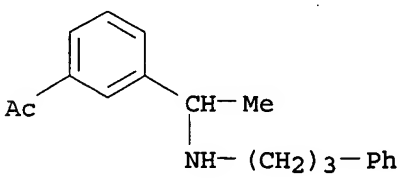
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6211244	B1	20010403	US 1995-546998	19951023

PRIORITY APPLN. INFO.: US 1995-546998 19951023
OTHER SOURCE(S): MARPAT 134:280612
GI

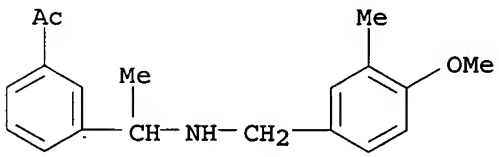


AB Title compds., e.g., I [R = H or alkyl; R1,R2 = (un)substituted Ph or naphthyl; Z = (CH2)0-3] were prepared Thus, (R)-1-(1-naphthyl)ethylamine was condensed with 2-acetonaphthone to give I (R = Me, R1 = 2-naphthyl, R2 = 1-naphthyl, Z = bond). Data for biol. activity of title compds. were given.
IT 159150-28-4P 332078-81-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1-arylethylamines as calcium receptor ligands)
RN 159150-28-4 CAPLUS
CN Ethanone, 1-[3-[1-[(3-phenylpropyl)amino]ethyl]phenyl]- (9CI) (CA INDEX

NAME)



RN 332078-81-6 CAPLUS
CN Ethanone, 1-[3-[1-[[(4-methoxy-3-methylphenyl)methyl]amino]ethyl]phenyl]-(9CI) (CA INDEX NAME)



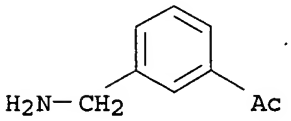
REFERENCE COUNT: 229 THERE ARE 229 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:523449 CAPLUS
DOCUMENT NUMBER: 133:281719
TITLE: Anti-Helicobacter pylori Agents. 4. 2-(Substituted guanidino)-4-phenylthiazoles and Some Structurally Rigid Derivatives
AUTHOR(S): Katsura, Yousuke; Tomishi, Tetsuo; Inoue, Yoshikazu; Sakane, Kazuo; Matsumoto, Yoshimi; Morinaga, Chizu; Ishikawa, Hirohumi; Takasugi, Hisashi
CORPORATE SOURCE: Medicinal Chemistry Research Laboratories and Medicinal Biology Research Laboratories, Fujisawa Pharmaceutical Company Ltd., Osaka, 532-8514, Japan
SOURCE: Journal of Medicinal Chemistry (2000), 43(17), 3315-3321
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:281719

AB In order to find a new class of anti-Helicobacter pylori (H. pylori) agents, a series of 4-[(3-acetamido)phenyl]-2-(substituted guanidino)thiazoles and some structurally rigid analogs were synthesized and evaluated for antimicrobial activity against H. pylori. Among the compds. obtained, high anti-H. pylori activities were observed in N-[[3-[2-[[imino[(phenylmethyl)amino]methyl]amino]-4-thiazolyl]phenyl]methyl]acetamide (MIC = 0.025 μg/mL) and N-[[3-[2-[[imino[(2-phenylethyl)amino]methyl]amino]-4-thiazolyl]phenyl]methyl]acetamide (MIC = 0.037 μg/mL) and N-[[3-[2-[[imino[[2-(2-methoxyphenyl)ethyl]amino]methyl]amino]-4-thiazolyl]phenyl]methyl]acetamide (MIC = 0.017 μg/mL). Though alkyl derivs. generally showed lower activity, N-[[3-[2-[[imino[(2-methoxyethyl)amino]methyl]amino]-4-thiazolyl]phenyl]methyl]acetamide preserved significant activity (MIC = 0.32 μg/mL) and also exhibited more potent gastric antisecretory activity than ranitidine. Structural restriction by bridging between the thiazole and the Ph rings with an alkyl chain did not improve the activity in this series.

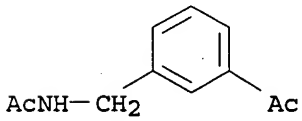
IT 149889-64-5P 149917-34-0P, N-[(3-Acetylphenyl)methyl]acetamide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (guanidino)phenylthiazoles and structurally rigid derivs. for inhibition of Helicobacter pylori)

RN 149889-64-5 CAPLUS
CN Ethanone, 1-[3-(aminomethyl)phenyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 149917-34-0 CAPLUS
CN Acetamide, N-[(3-acetylphenyl)methyl]- (9CI) (CA INDEX NAME)

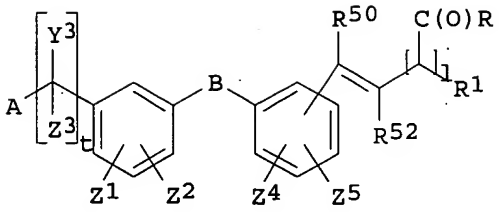


REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

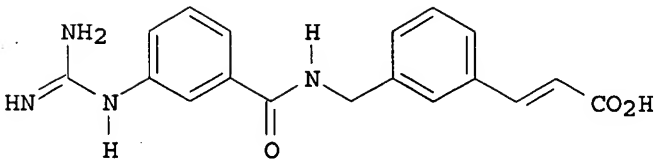
L15 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:12345 CAPLUS
DOCUMENT NUMBER: 130:81288
TITLE: Preparation of cinnamic acid derivatives for selective inhibiting or antagonizing the αvβ3 integrin
INVENTOR(S): Chen, Barbara B.; Chen, Helen Y.; Clare, Michael; Docter, Stephen H.; Khanna, Ish Kumar; Koszyk, Francis Jan; Malecha, James W.; Miyashiro, Julie Marion; Penning, Thomas D.; Rico, Joseph G.; Ruminski, Peter G.; Russell, Mark A.; Weier, Richard Mathias; Xu, Xiangdong; Yu, Stella S.; Yu, Yi
PATENT ASSIGNEE(S): G.D. Searle and Co., USA
SOURCE: U.S., 77 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5852210	A	19981222	US 1997-825080	19970327

PRIORITY APPLN. INFO.: US 1997-825080 19970327
OTHER SOURCE(S): MARPAT 130:81288
GI



I



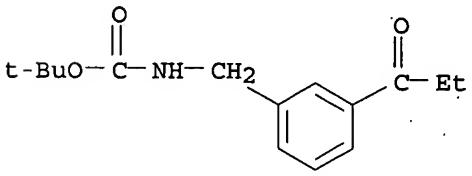
II

AB The title compds. [I; A = NR5C(:Y1)NR7R8 (wherein Y1 = NR2, O, S; R2 = H, alkyl, aryl, etc.; R7 = H, alkyl, alkenyl, etc.; R5 = H, alkyl, alkenyl, etc.; NR7R8 = (un)substituted 4-12 membered monocyclic or bicyclic ring containing 1 N atom), NR5C(Y2):NR7 (wherein Y2 = alkyl, cycloalkyl, bicycloalkyl, etc.), etc.; Z1, Z2, Z4, Z5 = H, alkyl, OH, etc.; B = CH:CH, CH2CONH, C(O)C:C, etc.; l = 0-3; t = 0-2; R50 = H, alkyl, aryl, etc.; R = XR3 (wherein X = O, S, NR4; R3, R4 = H, alkyl, alkenyl, etc.); Y3, Z3 = H, alkyl, aryl, etc.; R1 = H, alkyl, NH2, etc.; R52 = H, NHCO2R12, NSO2R12, etc.; R12 = H, alkyl, cycloalkyl, etc.] which selectively inhibit or antagonize the αvβ3 integrin, and are useful in treating tumor metastasis, solid tumor growth, angiogenesis, osteoporosis, humoral hypercalcemia of malignancy, smooth muscle cell migration, and restenosis, were prepared Thus, a 5-step synthesis of II, starting with 3-bromobenzylamine.HCl, which showed IC50 of 13.0 nM against αvβ3 vs. IC50 of 657 nM against IIb/IIIa.

IT 198195-10-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cinnamic acid derivs. for selective inhibiting or antagonizing the αvβ3 integrin)

RN 198195-10-7 CAPLUS

CN Carbamic acid, [[3-(1-oxopropyl)phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:338370 CAPLUS
DOCUMENT NUMBER: 129:27906
TITLE: Inhibitors of Acyl-CoA:Cholesterol O-Acyltransferase. Part 2. Identification and Structure-Activity Relationships of a Novel Series of N-Alkyl-N-(heteroaryl-substituted benzyl)-N'-arylureas

AUTHOR(S): Tanaka, Akira; Terasawa, Takeshi; Hagihara, Hiroyuki; Sakuma, Yuri; Ishibe, Noriko; Sawada, Masae; Takasugi, Hisashi; Tanaka, Hirokazu

CORPORATE SOURCE: Medicinal Chemistry Research Laboratories, Fujisawa Pharmaceutical Co. Ltd., Osaka, 532, Japan

SOURCE: Journal of Medicinal Chemistry (1998), 41(13), 2390-2410
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

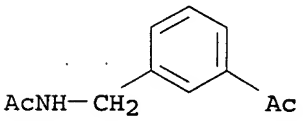
LANGUAGE: English

AB A series of N-alkyl-N-(heteroaryl-substituted benzyl)-N'-arylurea and related derivs. have been prepared and evaluated for their ability to inhibit acyl-CoA:cholesterol O-acyltransferase in vitro and to lower plasma cholesterol levels in cholesterol-fed rats in vivo. A pyrazol-3-yl group on the N-benzyl group was identified as a heteroarom. ring providing a good profile of biol. activity. As a result of optimization of the combination with the N-alkyl group and N-aryl group, compound FR186054 was identified as a new, orally efficacious ACAT inhibitor, which exhibited potent in vitro ACAT inhibitory activity (rabbit intestinal microsomes IC50 = 99 nM) and excellent hypocholesterolemic effects in cholesterol-fed rats, irresp. of administration mode (ED50 = 0.046 mg/kg dosed via the diet, ED50 = 0.44 mg/kg administered by gavage in PEG400 vehicle). Moreover, a toxicol. study revealed this compound to be nontoxic to the adrenal glands of dogs when tested at a single dose of 10 mg/kg po.

IT 149917-34-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of alkyl(heteroaryl-substituted benzyl)arylureas as acyl-CoA:cholesterol O-acyltransferase inhibitors)

RN 149917-34-0 CAPLUS

CN Acetamide, N-[(3-acetylphenyl)methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:455768 CAPLUS

DOCUMENT NUMBER: 125:114322

TITLE: Preparation of urea derivatives as cholesterol acyltransferase inhibitors

INVENTOR(S): Terasawa, Takeshi; Tanaka, Akira; Chiba, Toshiyuki; Takasugi, Hisashi

PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 228 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9610559	A1	19960411	WO 1995-JP1982	19950929
W: AU, CA, CN, HU, JP, KR, MX, RU, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2200981	AA	19960411	CA 1995-2200981	19950929

AU 9535779	A1	19960426	AU 1995-35779		19950929
EP 784612	A1	19970723	EP 1995-932934		19950929
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE					
JP 10510512	T2	19981013	JP 1995-511616		19950929
ZA 9508365	A	19960508	ZA 1995-8365		19951004
PRIORITY APPLN. INFO.:			GB 1994-19970	A	19941004
			GB 1995-6720	A	19950331
			GB 1995-14021	A	19950710
			WO 1995-JP1982	W	19950929

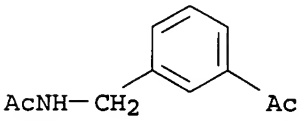
OTHER SOURCE(S): MARPAT 125:114322

AB R4YC6H4(CH2)nNR2CONHR3 [R2 = (ar)alkyl, heterocyclyl(alkyl), alkoxyalkyl, etc.; R3,R4 = (un)substituted aryl, heterocyclyl; Y = bond, alkylene, O, CO, CONH, etc.; n = 0 or 1] were prepare Thus, 1-cycloheptyl-1-(4-phenoxyphenylmethyl)-3-(2,4,6-trifluorophenyl)urea had IC50 of 1.1x10-8M against cholesterol acyltransferase in vitro.

IT 149917-34-0, N-(3-Acetylbenzyl)acetamide
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of urea derivs. as cholesterol acyltransferase inhibitors)

RN 149917-34-0 CAPLUS

CN Acetamide, N-[(3-acetylphenyl)methyl]- (9CI) (CA INDEX NAME)



L15 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:392101 CAPLUS

DOCUMENT NUMBER: 125:96084

TITLE: Aromatic compounds containing basic and acidic termini useful as fibrinogen receptor antagonists

INVENTOR(S): Cain, Gary A.; Eyermann, Charles J.

PATENT ASSIGNEE(S): Du Pont Merck Pharmaceutical Co., USA

SOURCE: U.S., 43 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 5523302	A	19960604	US 1993-157860		19931124
US 5739163	A	19980414	US 1996-612597		19960308
PRIORITY APPLN. INFO.:			US 1993-157860	A3	19931124

OTHER SOURCE(S): MARPAT 125:96084

AB This invention relates to novel compds. containing basic and acidic termini, pharmaceutical compns. containing such compds., processes for preparing such compds., and methods of using these compds., alone or in combination with other therapeutic agents, for the inhibition of platelet aggregation, as thrombolytics, and/or for the treatment of thromboembolic disorders.

IT 179002-56-3P 179002-58-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(aromatic compds. containing basic and acidic termini useful as fibrinogen receptor antagonists)

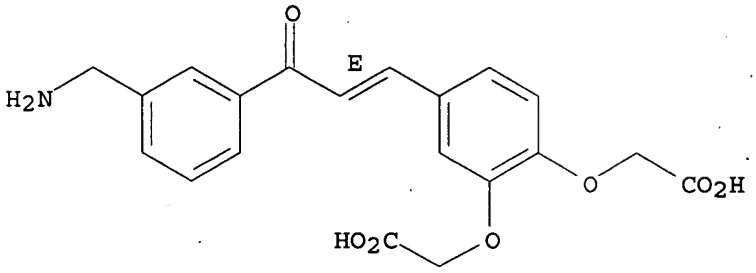
RN 179002-56-3 CAPLUS

CN Acetic acid, 2,2'-[[4-[3-[3-(aminomethyl)phenyl]-3-oxo-1-propenyl]-1,2-phenylene]bis(oxy)]bis-, (E)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

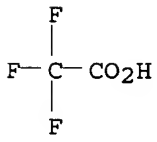
CRN 179000-32-9
CMF C20 H19 N O7

Double bond geometry as shown.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

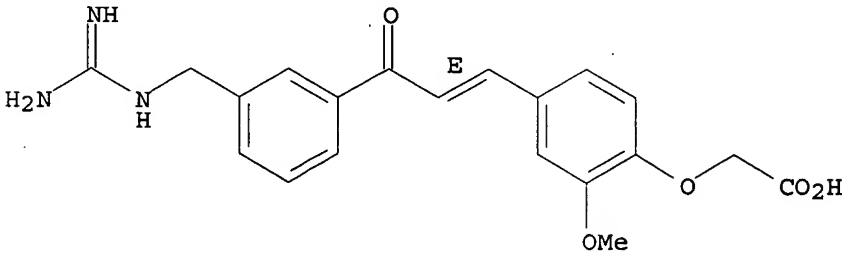


RN 179002-58-5 CAPLUS
CN Acetic acid, [4-[3-[3-[[(aminoiminomethyl)amino]methyl]phenyl]-3-oxo-1-propenyl]-2-methoxyphenoxy]-, (E)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

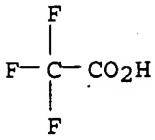
CRN 179000-68-1
CMF C20 H21 N3 O5

Double bond geometry as shown.



CM 2

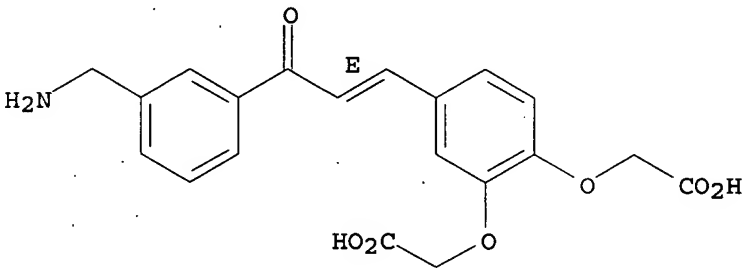
CRN 76-05-1
CMF C2 H F3 O2



IT 179000-32-9 179000-33-0 179000-34-1
179000-35-2 179000-36-3 179000-37-4
179000-41-0 179000-42-1 179000-43-2
179000-44-3 179000-68-1 179000-69-2
179000-70-5 179000-91-0 179002-51-8
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(aromatic compds. containing basic and acidic termini useful as fibrinogen receptor antagonists)

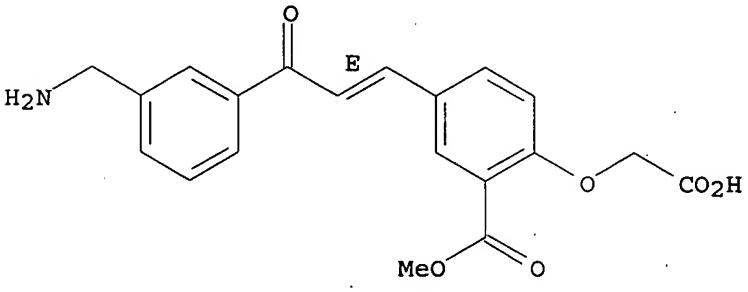
RN 179000-32-9 CAPLUS
CN Acetic acid, 2,2'-[[4-[3-[3-(aminomethyl)phenyl]-3-oxo-1-propenyl]-1,2-phenylene]bis(oxy)]bis-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



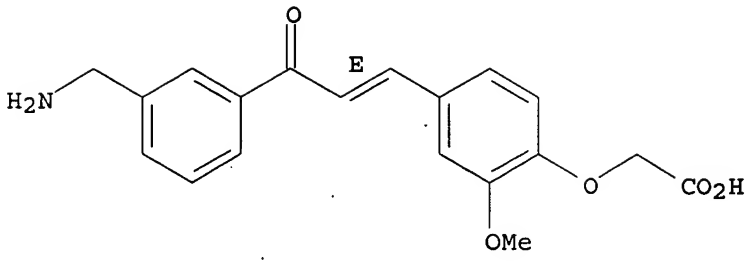
RN 179000-33-0 CAPLUS
CN Benzoic acid, 5-[3-[3-(aminomethyl)phenyl]-3-oxo-1-propenyl]-2-(carboxymethoxy)-, 1-methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



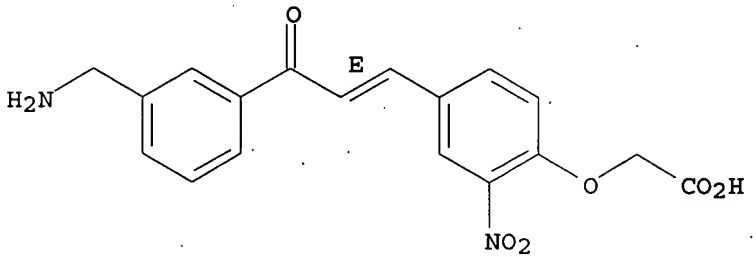
RN 179000-34-1 CAPLUS
CN Acetic acid, [4-[3-[3-(aminomethyl)phenyl]-3-oxo-1-propenyl]-2-methoxyphenoxy]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



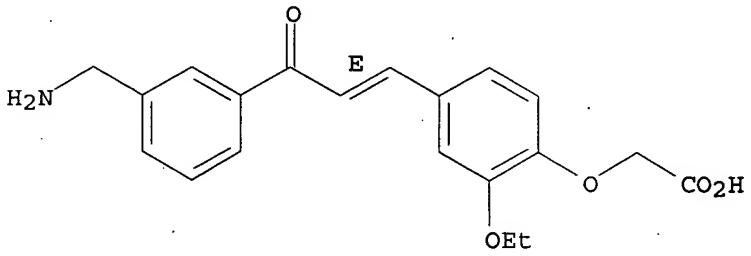
RN 179000-35-2 CAPLUS
CN Acetic acid, [4-[3-[3-(aminomethyl)phenyl]-3-oxo-1-propenyl]-2-nitrophenoxy]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



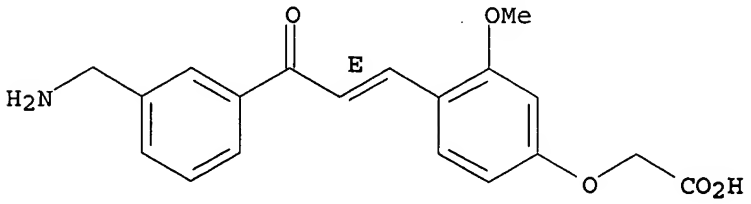
RN 179000-36-3 CAPLUS
CN Acetic acid, [4-[3-[3-(aminomethyl)phenyl]-3-oxo-1-propenyl]-2-ethoxyphenoxy]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



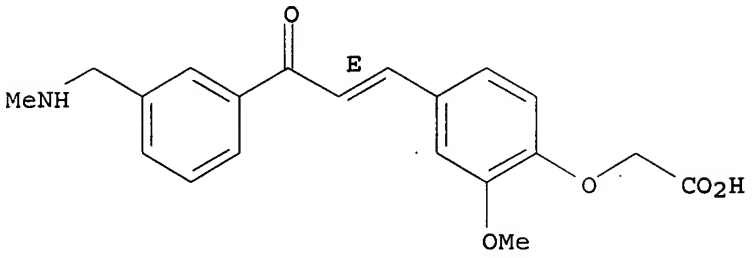
RN 179000-37-4 CAPLUS
CN Acetic acid, [4-[3-[3-(aminomethyl)phenyl]-3-oxo-1-propenyl]-3-methoxyphenoxy]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



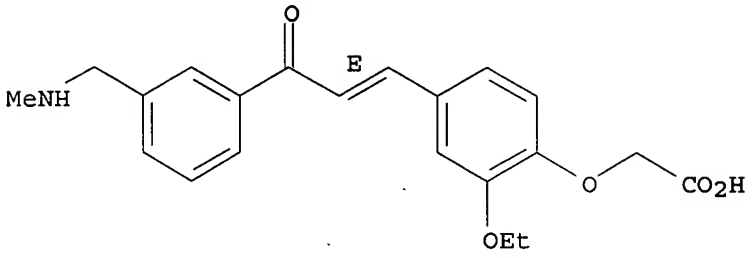
RN 179000-41-0 CAPLUS
CN Acetic acid, [2-methoxy-4-[3-[3-[(methylamino)methyl]phenyl]-3-oxo-1-propenyl]phenoxy]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



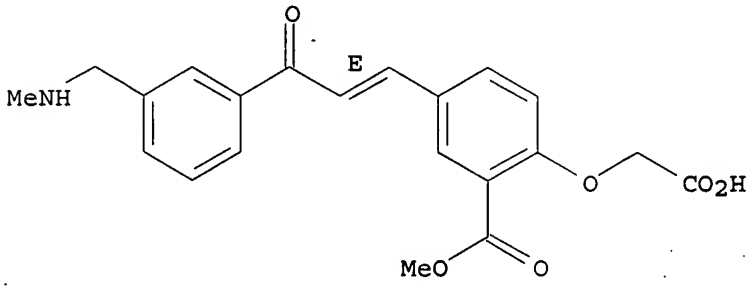
RN 179000-42-1 CAPLUS
CN Acetic acid, [2-ethoxy-4-[3-[3-[(methylamino)methyl]phenyl]-3-oxo-1-propenyl]phenoxy]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



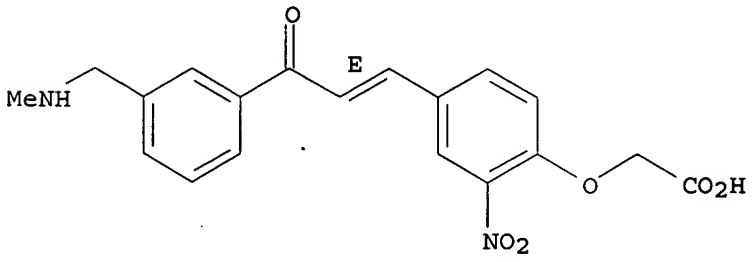
RN 179000-43-2 CAPLUS
CN Benzoic acid, 2-(carboxymethoxy)-5-[3-[3-[(methylamino)methyl]phenyl]-3-oxo-1-propenyl]-, 1-methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



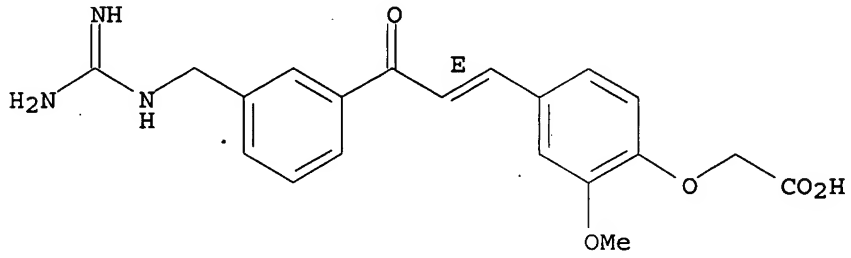
RN 179000-44-3 CAPLUS
CN Acetic acid, [4-[3-[3-[(methylamino)methyl]phenyl]-3-oxo-1-propenyl]-2-nitrophenoxy]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



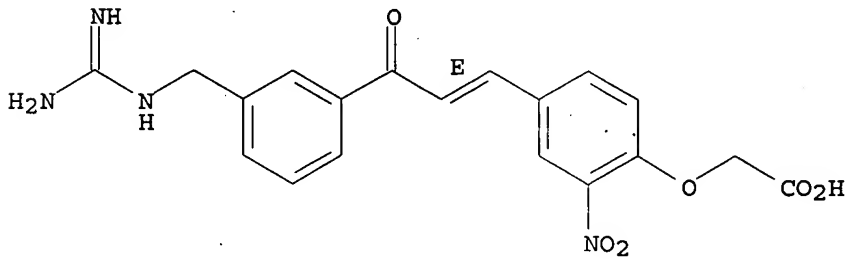
RN 179000-68-1 CAPLUS
CN Acetic acid, [4-[3-[3-[[(aminoiminomethyl)amino]methyl]phenyl]-3-oxo-1-propenyl]-2-methoxyphenoxy]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



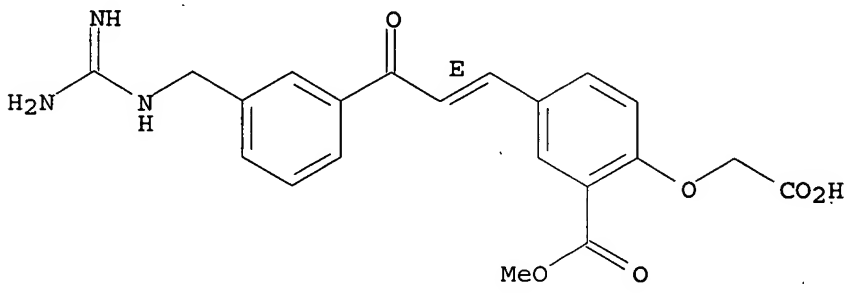
RN 179000-69-2 CAPLUS
CN Acetic acid, [4-[3-[3-[[(aminoiminomethyl)amino]methyl]phenyl]-3-oxo-1-propenyl]-2-nitrophenoxy]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

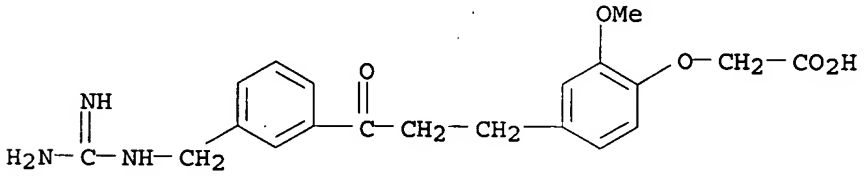


RN 179000-70-5 CAPLUS
CN Benzoic acid, 5-[3-[3-[[(aminoiminomethyl)amino]methyl]phenyl]-3-oxo-1-propenyl]-2-(carboxymethoxy)-, 1-methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

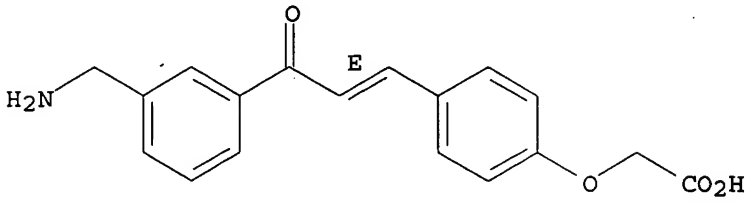


RN 179000-91-0 CAPLUS
CN Acetic acid, [4-[3-[3-[[(aminoiminomethyl)amino]methyl]phenyl]-3-oxopropyl]-2-methoxyphenoxy]- (9CI) (CA INDEX NAME)



RN 179002-51-8 CAPLUS
CN Acetic acid, [4-[3-[3-(aminomethyl)phenyl]-3-oxo-1-propenyl]phenoxy]-, (E)- (9CI) (CA INDEX NAME)

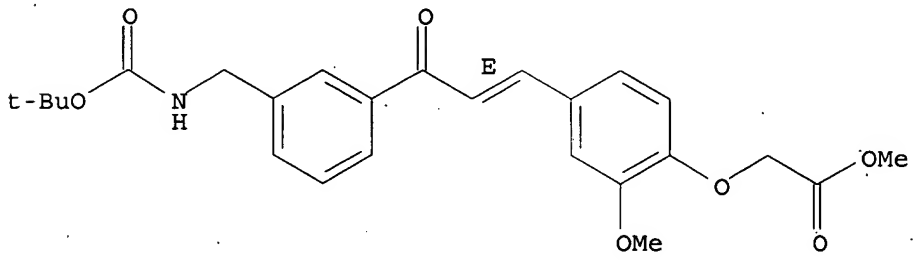
Double bond geometry as shown.



IT 179003-03-3P 179003-05-5P 179003-06-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(aromatic compds. containing basic and acidic termini useful as fibrinogen receptor antagonists)

RN 179003-03-3 CAPLUS
CN Acetic acid, [4-[3-[3-[[[(1,1-dimethylethoxy)carbonyl]amino]methyl]phenyl]-3-oxo-1-propenyl]-2-methoxyphenoxy]-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

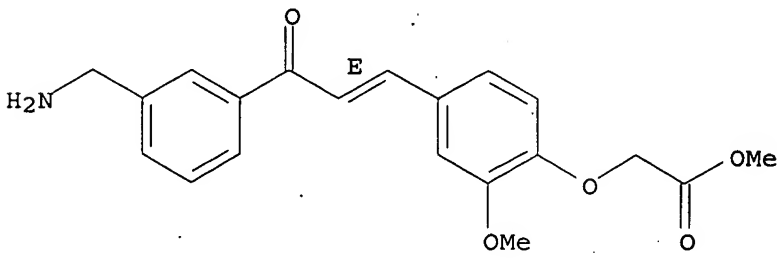


RN 179003-05-5 CAPLUS
CN Acetic acid, [4-[3-[3-(aminomethyl)phenyl]-3-oxo-1-propenyl]-2-methoxyphenoxy]-, methyl ester, (E)-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

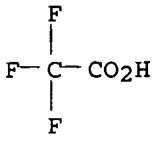
CRN 179003-04-4
CMF C20 H21 N O5

Double bond geometry as shown.



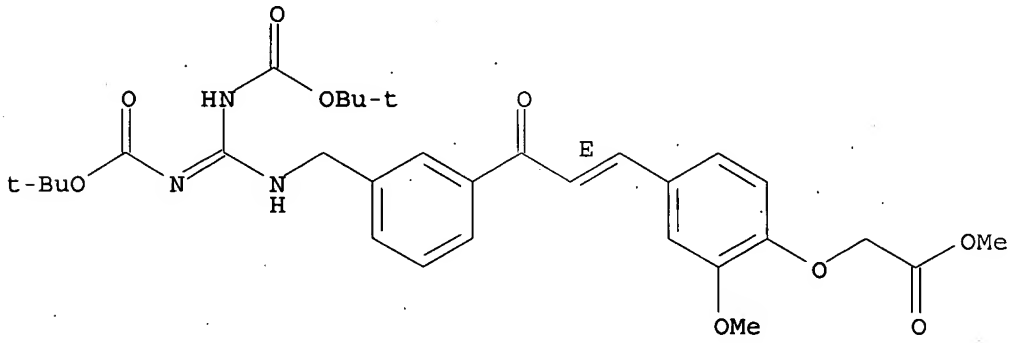
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 179003-06-6 CAPLUS
CN Acetic acid, [4-[3-[3-[[[bis[[(1,1-dimethylethoxy)carbonyl]amino]methylene]amino]methyl]phenyl]-3-oxo-1-propenyl]-2-methoxyphenoxy]-, methyl ester, (E)- (9CI) (CA INDEX NAME)

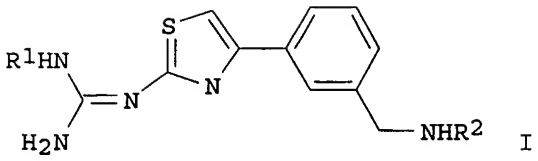
Double bond geometry as described by E or Z.



L15 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:385930 CAPLUS
DOCUMENT NUMBER: 125:58498
TITLE: Preparation of 4-(3-aminomethylphenyl)-2-thiazolylguanidines as H2-receptor antagonists
INVENTOR(S): Katsura, Yousuke; Tomishi, Tetsuo; Nishino, Shigetaka; Ohno, Mitsuko
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9605187	A1	19960222	WO 1995-JP1596		19950809
W: AU, BR, CA, CN, FI, HU, JP, KR, MX, NO, NZ, RU, UA, US					
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
AU 9531929	A1	19960307	AU 1995-31929		19950809
JP 2000504305	T2	20000411	JP 1995-507193		19950809
PRIORITY APPLN. INFO.:			GB 1994-16459	A	19940815
			WO 1995-JP1596	W	19950809

OTHER SOURCE(S): MARPAT 125:58498
GI



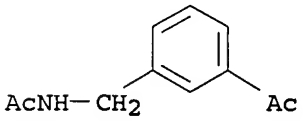
I

AB Title compds. [I; R1 = alkoxy(alkyl), cyanoalkyl, phenyl(oxy)(alkyl), etc.; R2 = H, alkanoyl, CONH2] were prepared Thus, I [R1 = 2-(1-cyclohexenyl)ethyl, R2 = Ac] gave 100% inhibition of histamine-induced increase of guinea pig atrial strip contraction at 10-6g/mL in vitro.

IT 149917-34-0, 3-(Acetylaminomethyl)acetophenone
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 4-(3-aminomethylphenyl)-2-thiazolylguanidines as H2-receptor antagonists)

RN 149917-34-0 CAPLUS

CN Acetamide, N-[(3-acetylphenyl)methyl]- (9CI) (CA INDEX NAME)



L15 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:934019 CAPLUS

DOCUMENT NUMBER: 123:340105

TITLE: Preparation of oxazole derivatives as bactericides and ulcer inhibitors

INVENTOR(S): Katsura, Yosuke; Inoe, Zenichi; Fuji, Tetsuo; Takasugi, Hisashi

PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

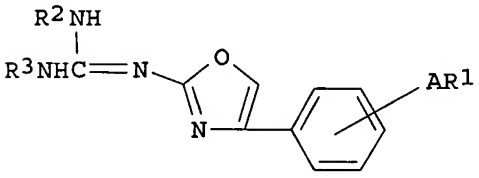
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
JP 07188197	A2	19950725	JP 1994-303222		19941110
PRIORITY APPLN. INFO.:			JP 1994-303222	A	19941110
			JP 1993-312542		19931117

OTHER SOURCE(S): MARPAT 123:340105

GI



I

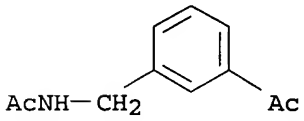
AB The title compds. I [R1 = (un)substituted amino; R2, R3 = H, (un)substituted aliphatic hydrocarbon, etc.; A = alkylene] are prepared

4-(3-Acetylaminomethylphenyl)-2-[(amino)(2-methoxybenzylamino)methyleneamino]oxazole (preparation given) in vitro showed MIC of 0.182 μg/mL against Helicobacter Pylori. The MICs of 3 three other compds. of this invention against Helicobacter Pylori are also given this document.

IT 149917-34-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of oxazole derivs. as bactericides and ulcer inhibitors)

RN 149917-34-0 CAPLUS

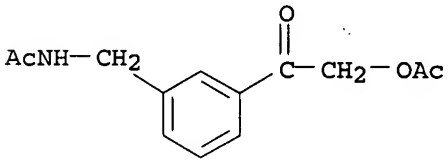
CN Acetamide, N-[(3-acetylphenyl)methyl]- (9CI) (CA INDEX NAME)



IT 170634-23-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of oxazole derivs. as bactericides and ulcer inhibitors)

RN 170634-23-8 CAPLUS

CN Acetamide, N-[[3-[(acetyloxy)acetyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



L15 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:436152 CAPLUS

DOCUMENT NUMBER: 121:36152

TITLE: Template-Constrained Cyclic Peptides: Design of High-Affinity Ligands for GPIIb/IIIa

AUTHOR(S): Jackson, Sharon; DeGrado, W.; Dwivedi, A.; Parthasarathy, A.; Higley, A.; Krywko, J.; Rockwell, A.; Markwalder, J.; Wells, G.; et al.

CORPORATE SOURCE: Experimental Station, DuPont Merck Pharmaceutical Company, Wilmington, DE, 19880-0328, USA

SOURCE: Journal of the American Chemical Society (1994), 116(8), 3220-30
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

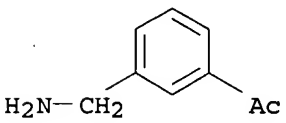
AB The general strategy of tying amino and carboxy terminal ends of a peptide onto a semirigid template to lock the intervening peptide backbone into a single conformer or a family of related conformers was tested using the tripeptide sequence Arg-Gly-Asp (RGD), which binds with low affinity to the platelet glycoprotein IIb/IIIa (GPIIb/IIIa). Mimics of RGD are of interest as antithrombotics because of their ability to inhibit the aggregation of platelets. Prior to this study, J. Samanen; et al. (1991) prepared disulfide-containing cyclic pentapeptide I (MeArg = N-methyl-L-arginine, Pen = L-penicillamine) (SK&F 106760) that bound to GPIIb/IIIa with an affinity of approx. 0.1 μM. NMR anal. of the solution conformation of I suggested that replacing the disulfide-containing portion of the cycle with m-(aminomethyl)benzoic acid would lead to a more rigid structure. 39Indeed, introduction of this template into a cyclic RGD-containing peptide resulted in compds. with high affinity for the

receptor. Further, systematic inclusion of addnl. conformational constraints in the form of Nα- and Cα-alkyl groups led to peptide II with an affinity of approx. 100 pM for binding to the receptor. II also showed good activity in the platelet aggregation assay at oral doses as low as 0.1 mg/kg.

IT 149889-64-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and butoxycarbonylation of)

RN 149889-64-5 CAPLUS

CN Ethanone, 1-[3-(aminomethyl)phenyl]-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

L15 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:603405 CAPLUS

DOCUMENT NUMBER: 119:203405

TITLE: Preparation of guanidinothiazoles and their use as histamine H2-receptor antagonists

INVENTOR(S): Katsura, Yousuke; Tomishi, Tetsuo; Inoue, Yoshikazu; Takasugi, Hisashi

PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan

SOURCE: Eur. Pat. Appl., 49 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 545376	A1	19930609	EP 1992-120533	19921202
EP 545376	B1	19980909		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
ZA 9208876	A	19930715	ZA 1992-8876	19921117
AU 9229837	A1	19930610	AU 1992-29837	19921202
AU 666893	B2	19960229		
JP 06321921	A2	19941122	JP 1992-323052	19921202
JP 2531329	B2	19960904		
AT 170851	E	19980915	AT 1992-120533	19921202
CA 2084640	AA	19930607	CA 1992-2084640	19921204
HU 65776	A2	19940728	HU 1992-3849	19921204
CN 1079469	A	19931215	CN 1992-114939	19921205
US 5532258	A	19960702	US 1994-356967	19941216
PRIORITY APPLN. INFO.:			GB 1991-25970 A	19911206
			US 1992-978477 B1	19921118

OTHER SOURCE(S): MARPAT 119:203405

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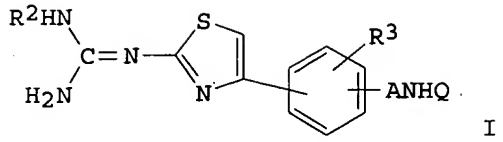

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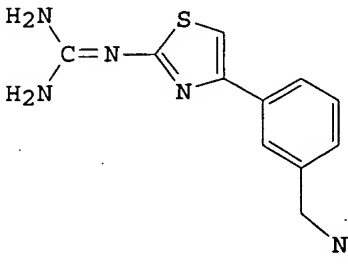
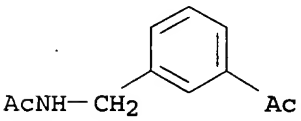


II

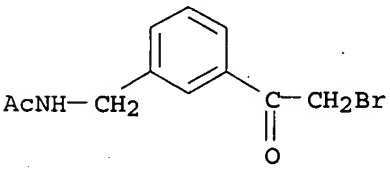
AB Title compds. [I; R2 = H, (substituted) alkyl; R3 = H, alkyl, alkoxy, halo; A = alkylene; Q = COR1, (substituted) carbamimidoyl; R1 = organic group], were prepared Thus, 4-(3-aminomethylphenyl)-2-(diaminomethyleneamino)thiazole dihydrochloride (preparation given) was stirred with potassium isocyanate in H2O at room temperature for 8.5 h to give title compound II. II at 1 mg/kg i.v. in rats inhibited 99% gastric acid secretion.

IT 149917-34-0P 149917-44-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for guanidinothiazole derivative hiatamine receptor H2 antagonist)

RN 149917-34-0 CAPLUS
CN Acetamide, N-[(3-acetylphenyl)methyl]- (9CI) (CA INDEX NAME)

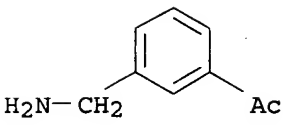


RN 149917-44-2 CAPLUS
CN Acetamide, N-[[3-(bromoacetyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



IT 149889-64-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of guanidinothiazole H2 antagonist)

RN 149889-64-5 CAPLUS
CN Ethanone, 1-[3-(aminomethyl)phenyl]-, hydrochloride (9CI) (CA INDEX NAME)

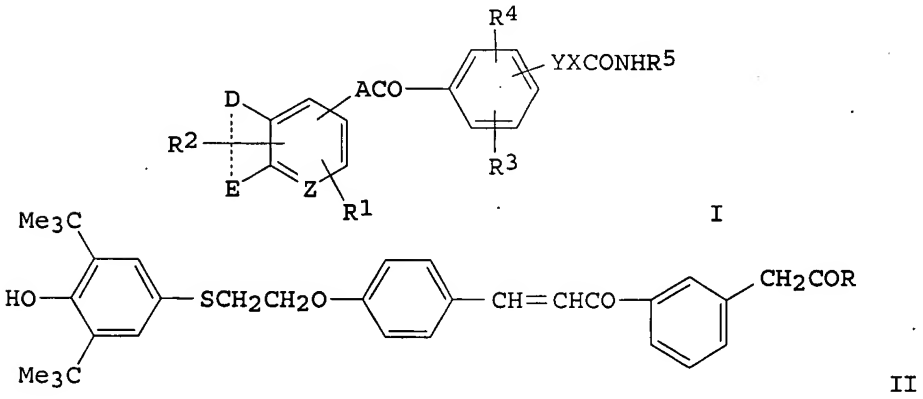


● HCl

L15 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:449076 CAPLUS
DOCUMENT NUMBER: 119:49076
TITLE: Preparation of phenylacetamide derivatives as acyl Co-A-cholesterol acyltransferase (ACAT) inhibitors
INVENTOR(S): Sano, Mitsuharu; Chihara, Yasuaki; Ikezawa, Ryuhei; Ooe, Takanori; Kusuhara, Hidenobu; Izumi, Noritaka
PATENT ASSIGNEE(S): Yoshitomi Pharmaceutical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05025115	A2	19930202	JP 1991-203857	19910717
PRIORITY APPLN. INFO.:			JP 1991-203857	19910717

OTHER SOURCE(S): CASREACT 119:49076; MARPAT 119:49076
GI



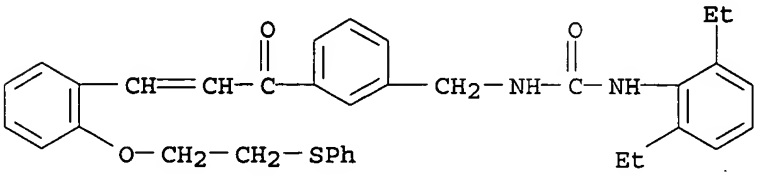
I

II

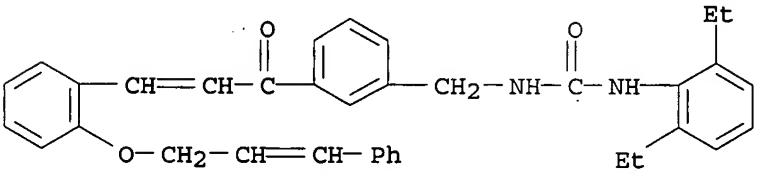
AB The title compds. [I; R1, R2 = H, halo, alkyl, alkoxy, aryloxy, aralkoxy, etc.; R3, R4 = H, halo, alkyl, alkoxy; R5 = (substituted) aryl; A = alkylene, alkenylene; Z = CH, N; Y = alkylene, oxyalkylene; X = bond, NH; DE may form a ring], useful as anticholesteremics and arteriosclerotics, are prepared Et3N was added to a solution of acid II (R = OH) in EtOAc, followed by pivaloyl chloride with stirring at 0-5°, 2,6-Et2C6H3NH2 was added at 0-5°, and the mixture was stirred at room temperature to give amide II (R = 2,6-Et2C6H3NH). Also prepared were 27 addnl. I, which showed IC50 of 0.02-0.07 μM against ACAT and lowered liver cholesterol by 35-61% in rats at 0.01-0.1% in feed.

IT 148491-56-9P 148491-58-1P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as anticholesteremic and arteriosclerotic agent)
RN 148491-56-9 CAPLUS
CN Urea, N-(2,6-diethylphenyl)-N'-[[3-[1-oxo-3-[2-[2-(phenylthio)ethoxy]phenyl]-2-propenyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



RN 148491-58-1 CAPLUS
CN Urea, N-(2,6-diethylphenyl)-N'-[[3-[1-oxo-3-[2-[(3-phenyl-2-propenyl)oxy]phenyl]-2-propenyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



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757 L3
955395 ALUMINUM
L16 3 L3 AND ALUMINUM

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L16 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:722822 CAPLUS
DOCUMENT NUMBER: 141:239312
TITLE: Compositions and methods for detection and isolation of phosphorylated molecules
INVENTOR(S): Agnew, Brian; Beechem, Joseph; Gee, Kyle; Haugland, Richard; Steinberg, Thomas; Patton, Wayne
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 89 pp., Cont.-in-part of U.S. Ser. No. 428,192.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004171034	A1	20040902	US 2003-703816	20031107
US 2004038306	A1	20040226	US 2003-428192	20030502
US 7102005	B2	20060905		
CA 2483868	AA	20040521	CA 2003-2483868	20030502
AU 2003299466	A1	20040607	AU 2003-299466	20030502
EP 1546118	A2	20050629	EP 2003-799756	20030502
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

JP 2005539243	T2	20051222	JP 2004-549877		20030502
US 2005014197	A1	20050120	US 2004-821522		20040409
WO 2005047901	A2	20050526	WO 2004-US36968		20041105
WO 2005047901	A3	20050728			

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

US 2002-377733P	P	20020503
US 2002-393059P	P	20020628
US 2002-407255P	P	20020830
US 2003-440252P	P	20030114
US 2003-428192	A2	20030502
WO 2003-US13765	W	20030502
US 2003-703816	A2	20031107

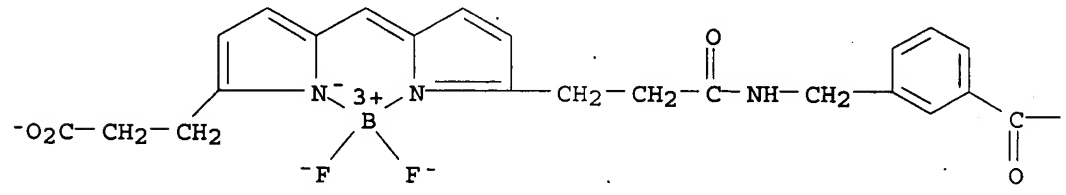
AB The present invention relates to phosphate-binding compds. that find use in binding, detecting and isolating phosphorylated target mols. including the subsequent identification of target mols. that interact with phosphorylated target mols. or mols. capable of being phosphorylated. A binding solution is provide that comprises a phosphate-binding compound, an acid and a metal ion wherein the metal ion simultaneously interacts with an exposed phosphate group on a target mol. and the metal chelating moiety of the phosphate-binding compound forming a bridge between the phosphate-binding compound and a phosphorylated target mol. resulting in a ternary complex. The binding solution of the present invention finds use in binding and detecting immobilized and solubilized phosphorylated target mols., isolation of phosphorylated target mols. from a complex mixture and aiding in proteomic anal. wherein kinase and phosphatase substrates and enzymes can be identified.

IT 749863-24-9P 749863-26-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(compns. and methods for detection and isolation of phosphorylated mols.)

RN 749863-24-9 CAPLUS

CN Borate(1-), [5-[[5-[3-[[(3-benzoylphenyl)methyl]amino]-3-oxopropyl]-2H-pyrrol-2-ylidene-κN]methyl]-1H-pyrrole-2-propanoato(2-)-κN1]difluoro-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)

PAGE 1-A



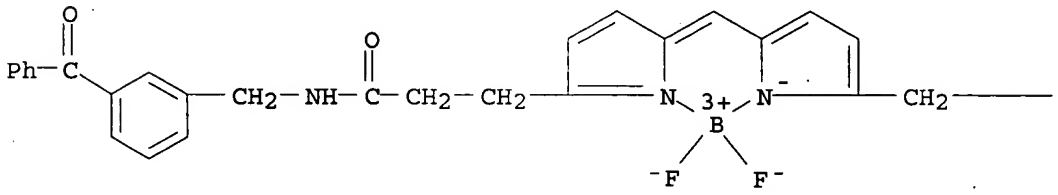
● H+

PAGE 1-B

— Ph

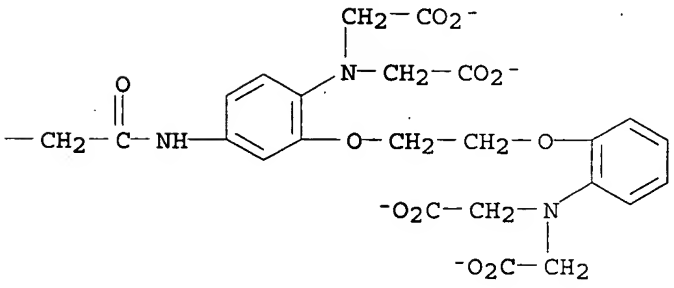
RN 749863-26-1 CAPLUS
CN Borate(4-), [N-[2-[2-[5-[[3-[5-[[5-[3-[[(3-benzoylphenyl)methyl]amino]-3-oxopropyl]-2H-pyrrol-2-ylidene-κN]methyl]-1H-pyrrol-2-yl-κN]-1-oxopropyl]amino]-2-[bis(carboxymethyl)amino]phenoxy]ethoxy]phenyl]-N-(carboxymethyl)glycinato(5-)]difluoro-, tetrasodium, (T-4)- (9CI) (CA INDEX NAME)

PAGE 1-A



● 4 Na^+

PAGE 1-B



L16 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	2004:610021 CAPLUS
DOCUMENT NUMBER:	141:153045
TITLE:	Fluorescent assays for screening for protein kinase inhibitors applicable in cancer treatment and diagnosis
INVENTOR(S):	Lawrence, David S.
PATENT ASSIGNEE(S):	Albert Einstein College of Medicine of Yeshiva University, USA
SOURCE:	PCT Int. Appl., 188 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004062475	A2	20040729	WO 2004-US480	20040109
WO 2004062475	A3	20050901		
W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GH, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR, KZ, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ				
US 2005054024	A1	20050310	US 2004-755086	20040109
PRIORITY APPLN. INFO.:			US 2003-439359P P	20030110
			US 2003-505097P P	20030922

OTHER SOURCE(S): MARPAT 141:153045

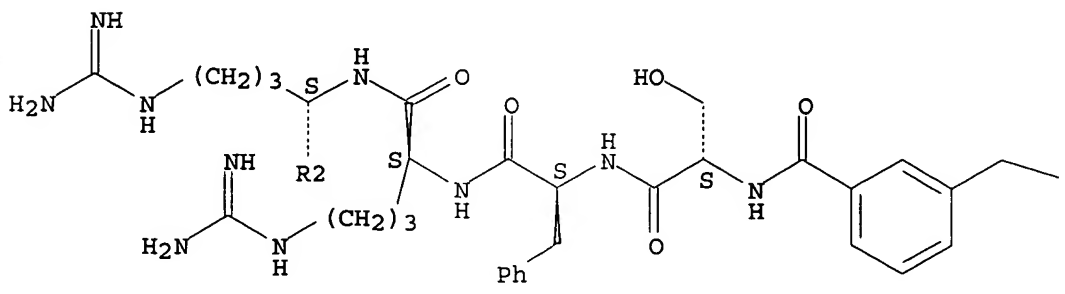
AB This invention provides fluorescently-labeled peptide substrates for protein kinases; methods using the substrates for identifying compds. that inhibit protein kinases, for determining if particular protein kinases are active in cells, for diagnosing diseases, and for preparing compns.; and compns. comprising the substrates. Several schemes for the synthesis of protein kinase C fluorescently-labeled peptide substrates, adaptable to the preparation of large peptide libraries, are provided. In particular embodiments, a library of fluorescently labeled protein kinase C (PKC) peptide substrates was prepared to identify a phosphorylation-induced reporter of protein kinase activity. The lead PKC substrate displays a 2.5-fold change in fluorescence intensity upon phosphorylation. PKC activity can also be detected in cell lysates containing the activated PKCs and living cells. Immunodepletion of conventional PKCs from the cell lysate eliminates the fluorescence response, suggesting that this peptide substrate is selectively phosphorylated by PKCα, β, and γ. Finally, living cells microinjected with the peptide substrate exhibit a 2-fold increase in fluorescence intensity upon exposure to a PKC activator. Thus this peptide based protein kinase biosensors is useful in monitoring the temporal and spatial dynamics of PKC activity in living cells, and applicable in cancer treatment and diagnosis.

IT 728044-64-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(fluorescent assays for screening for protein kinase inhibitors applicable in cancer treatment and diagnosis)

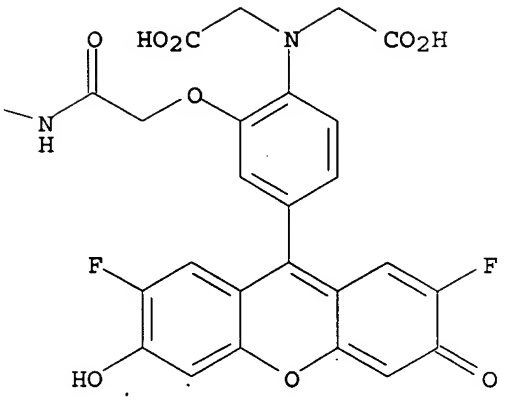
RN 728044-64-2 CAPLUS

CN L-Lysinamide, N-[3-[[[[2-[bis(carboxymethyl)amino]-5-(2,7-difluoro-6-hydroxy-3-oxo-3H-xanthen-9-yl)phenoxy]acetyl]amino]methyl]benzoyl]-L-seryl-L-phenylalanyl-L-arginyl-L-arginyl-L-arginyl-L-arginyl-N-(2-mercaptoethyl)- (9CI) (CA INDEX NAME)

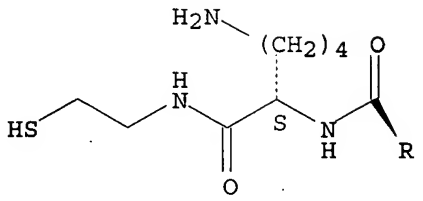
Absolute stereochemistry.

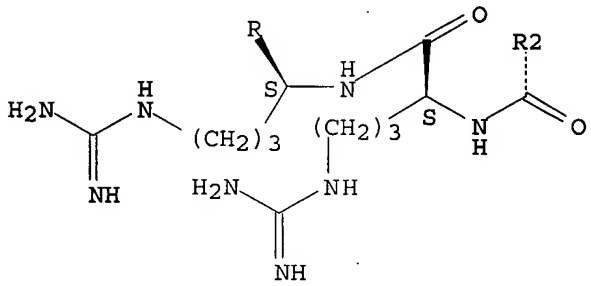


PAGE 1-B

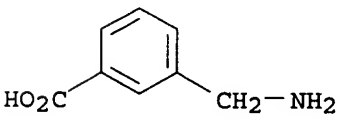


PAGE 2-A





IT 2393-20-6
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(linker in PKC peptide substrate; fluorescent assays for screening for protein kinase inhibitors applicable in cancer treatment and diagnosis)
RN 2393-20-6 CAPLUS
CN Benzoic acid, 3-(aminomethyl)- (9CI) (CA INDEX NAME)



L16 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN